

Research Activity: **Engineering Physics**
Division: Materials Sciences and Engineering
Primary Contact(s): Timothy Fitzsimmons (Tim.Fitzsimmons@science.doe.gov; 301-903-9830)
Team Leader: Robert J. Gottschall
Division Director: Harriet Kung

Portfolio Description:

Engineering Physics advances scientific understanding underlying the dynamic interactions of single and multicomponent solid and fluid systems. Research considers the behavior and interactions of fluids including organic, biological and complex fluids with each other and with solid systems; the transport of energy on and within these systems; and the development of means to advance the characterization of these systems. Issues under consideration frequently span several orders of magnitude in length and time scales and range from atomic interactions to macroscopic behavior and subpicosecond chemical events to fatigue events that may take years to reach completion. Accordingly they present a considerable challenge to theory, computational simulation and experiment. Questions of ongoing interest include understanding and predicting the behavior of (1) nanoscale structures and systems, including those with biological components; (2) dynamics of fluids, especially multi-component and complex fluids, but also including heat transfer, solidification and granular materials; and, (3) interactions of phonons with interfaces, secondary phases or with micro and nanoscale defects in solids. Opportunities of current and future interest include transport issues related to hydrogen storage and production, nano-motor design, thermal transport in nano-fluids.

Unique Aspects:

Engineering Physics has a unique role to play in National Nanotechnology and Hydrogen Initiatives to further the understanding of nano- and meso-structures, devices and systems; molecular machines; transport behavior to and within consolidated nano-particulate material; and the dynamic behavior of multiphase, complex and biologically inspired materials. This activity has and maintains a leadership role in the fundamental understanding of multiphase fluid flow, heat transfer, and in the fundamental behavior of granular materials.

Relationship to Others:

Interacts with the community through: (1) workshops such as the Workshop on Multiphase Fluid Flow, May, 2002 and the upcoming Symposium on Computational Approaches to Disperse Multiphase Flows, in October, 2004; (2) program presentations to the American Society of Mechanical Engineers, the American Society for Engineering Education and other groups.

Interacts with other agencies and interagency working groups such as: (1) NSF – Exploring potential joint interests in fluid flow and heat transfer (2) NSTC Interagency Working Group on Nanotechnology and (3) Interagency Coordinating Committee on Non-Destructive Evaluation.

Interfaces and coordinates with the Synthesis and Processing, Physical Behavior, Mechanical Behavior and Radiation Effects, and Condensed Matter Theory Core Research Activities. Work in droplets and sprays supports work in combustion which is funded in a number of other programs in the Department of Energy.

Collaborates with the Mathematical, Informational and Computational Sciences Division on work of mutual interest.

Significant Accomplishments:

- Development of a nanosized *biological* motor for use in MEMS and NEMS devices
- Creation of the first *synthetic* nanosized electric motor
- Research on nanomotion from biomolecular interactions has led to the development of instruments for detecting and identifying molecules
- Adding small quantities of carbon nanotubes to a fluid dramatically increases its ability to conduct heat, however, theory predicts an even larger increase in conductivity. Experiments and simulations point to poor thermal coupling between the nanotubes and the fluid with implications for designing advanced heat transfer systems.
- Thermal conductivity of single crystal silicon nanowires has been discovered to be two orders of magnitude lower than the bulk thermal conductivity of silicon, a highly desirable property for thermoelectric applications. Simultaneously, the results reveal their limitation for electronics and photonics applications.

- Record heat flux dissipation achieved with micro-channel two-phase flow (27,600 W/cm²).
- Oil and gas companies are using results of research for more efficient transport and exploration of crude oil and natural gas. The Syncrude pipeline, which yields a 97% saving in energy to transport the crude, would not have been built without these developments.

Mission Relevance:

Improved understanding of dynamic behavior at the nano- and micro-scale will advance sensing and control capabilities, lead to accurate predictions of materials and systems behavior, and enable larger-scale applications of devices with nano-scale components. Together these advances will further lead to higher process efficiency and lower energy consumption. Improving the knowledge base on multi-component fluid dynamics and heat transfer will have a major impact on energy consumption because these phenomena are an integral part of every industrial process. Potential impacts include improved efficiency of fossil and nuclear based power generating systems.

Scientific Challenges:

How can we accurately model the transport of hydrogen and heat through nanoscale materials, and nanoporous and mesoporous structures? What are the explanations for anomalous thermal behavior of nanofluids and nanowires? Where do the continuum approximations break down in multicomponent systems containing fluids? Can we adequately describe, simulate and engineer macroscale systems to take advantage of nanoscale behavior? Challenges include understanding: 1) the potential of chemical and biological systems to construct complex, nanostructured materials under ambient conditions; 2) the role of interfaces and structure on the behavior of simple and complex fluids; 3) how more realistic sized groupings of drops and bubbles interact with each other and with their environment; 4) the mechanics and energetics of molecular mechanical devices; 5) simple and complex systems driven far from thermodynamic equilibrium; and 6) the interactions of phonons with defects and interfaces.

Funding Summary:

Dollars in Thousands

<u>FY 2003</u>	<u>FY 2004</u>	<u>FY 2005 Request</u>
15,297	14,038	13,500

The program provides funding for 51 university grants, 13 programs at national laboratories, and 1 program in industry. Funding demographics is shown below:

<u>Performer</u>	<u>Funding Percentage</u>
DOE Laboratories	46%
Universities	52%
Other	2%

These are percentages of the operating research expenditures in this area; they do not contain laboratory capital equipment, infrastructure, or other non-operating components.

Projected Evolution:

The program will continue to refine its core of excellence in nanotechnology and microsystems, multi-component and complex fluid dynamics, granular materials, heat transfer, and other select areas such as phonon behavior. The program will increasingly pursue understanding of the dynamics of the solid-liquid interface, of multicomponent fluids at the micro- and nano-scale, and the interface and dynamics of organic and biological materials with fluids and solids.